

## 2. Basic Notions of Mixing and Turbulence

By mixing we understand the process of achieving a uniform composition by forced and random movement of fluid elements. Chemical reactions cause compositional differences in process vessels. Gross fluid motion reduces the scale over which such differences exist. Molecular diffusion reduces the intensity of the differences.

Thus we need to introduce two measures of the state of the system and consider their evolution in time or space.

Scale of segregation,  $L_s$ , is a measure of the average size of unmixed clumps of the original compositions e.g. pure components.

Intensity of segregation,  $I_s$ , is a measure of the difference in concentration between neighboring clumps of fluid.

The vector scale of segregation for spatially distributed mixtures of arbitrary complexity is given by

$$L_v = \int_0^{r_{\max}} g_v(\vec{r}) d(\vec{r}) \quad (1)$$

where  $r_{\max} = \max(\vec{r})$  allowed by the physical limitations on the apparatus, and  $g_v(\vec{r})$  is the vector correlation coefficient:

$$g_v(\vec{r}) = \frac{\sum (C(\vec{z}) - \bar{C})(C(\vec{z} + \vec{r}) - \bar{C})}{\sum (C(\vec{z}) - \bar{C})^2} \quad (2)$$

where the summation is taken over many points at various locations  $z$ . Then

$$\bar{C} = \frac{1}{N} \sum_N C(\vec{z}) \quad (3)$$

or in a continuous representation

$$g_v(\vec{r}) = \frac{\int (C(\vec{z}) - \bar{C})(C(\vec{z} + \vec{r}) - \bar{C}) dv}{\int (C(\vec{z}) - \bar{C})^2 dv} \quad (2a)$$

$$\bar{C} = \frac{1}{V} \int_V C(\vec{z}) dv \quad (3a)$$

where  $V$  is the volume of interest.

Clearly  $g_v(\vec{r})$  is a scalar function of a vector quantity and can in general depend on direction  $g_v(\vec{0}) \rightarrow 1$ , and for random mixtures  $g_v(|r| \rightarrow \infty) = 0$ . If a mixture has a regular structure then  $g_v(\vec{r})$  might be periodic in the appropriate direction.

The intensity of segregation for the whole system could be defined by:

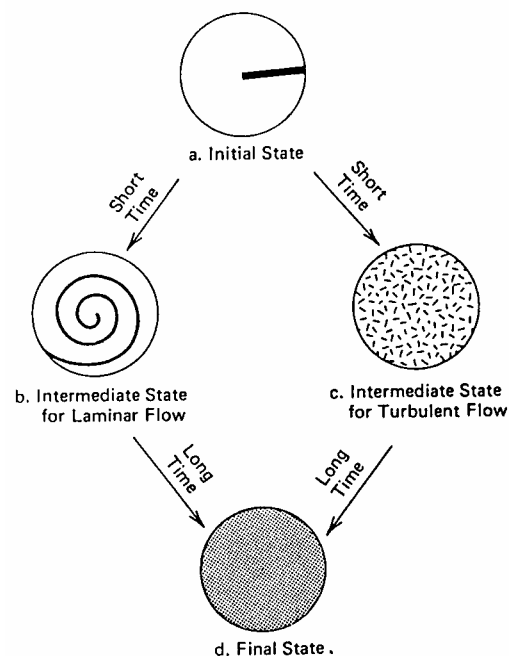
$$I_s = \frac{\frac{1}{V} \int_v (C(\bar{z}) - \bar{C})^2 dv}{\bar{C}^2} \quad (4)$$

Neither eq (2) or (4) are particularly useful because they would be extremely difficult to execute experimentally and yet  $L_v$  or  $I_s$  cannot be readily predicted. However, the question arises as to what one considers "a point" so that a point is still large enough for concentration to have meaning. We will see later how to reduce these quantities, based on a number of simplifying assumptions, to a usable form.

First, in Figure 1 we illustrate how mixing of an initially segregated state can reach a state of a homogenous mixture. Laminar mixing involves flow along welldefined streamlines and continuous folding (and in other flows also thinning) of the initial zone containing only material one (say dark stream in Figure 1). After some time has passed diffusion takes over to create a final state. However, the same type of initial mixing would happen in any inviscid flow, say irrotational flow where the tangential velocity within a circular element is  $u_t = \frac{\Gamma}{2\pi r}$ . Once the distance "striation thickness"

between stream lines containing material A (dark) which is mixed into material B (white) is reduced to a scale over which diffusion takes place rapidly diffusion ultimately takes over. If one would reverse the flow before diffusional effects are felt one would be able to reconstruct the starting condition of the material. This has been proven experimentally by G.I. Taylor. After diffusion takes over entropy of the system is increased and reversing the flow cannot bring the system to the original starting point.

**FIGURE 1:** Successive stages of a batch mixing process

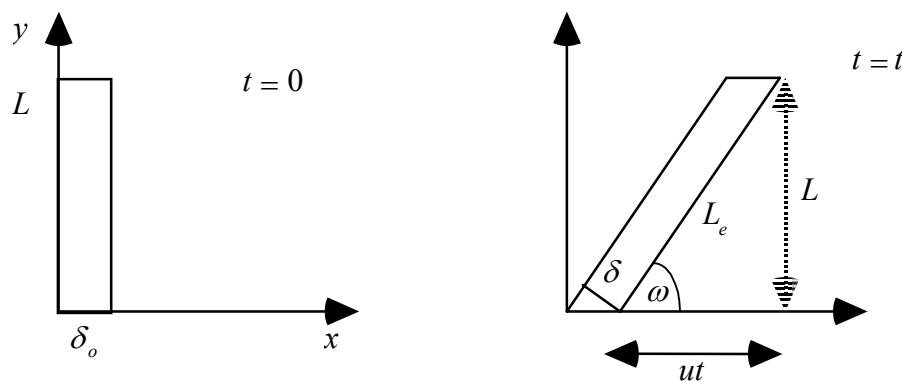


Turbulent mixing occurs by eddy motion. Turbulent fluid motion is an irregular condition of flow in which the various velocities, concentrations and other quantities show a random variation with time and space coordinates so that statistically distinct average values can be discerned. Turbulent motion consists of super-position of eddies of various sizes and vorticities with distinguishable upper and lower limits. The upper limit is determined by the size of the apparatus (its smallest dimension, usually). The lower limit is determined by viscous effects and decreases with the increase in the average velocity of flow (other conditions being the same). Within the smallest eddies the flow is viscous in nature ( $Re_{\text{eddy}} = O(1)$ ) and molecular momentum, mass and heat transport dominate. Still the continuum approach (also the notion of concentration, etc.) is justified even for the smallest eddies. In gases at  $\bar{u} = 100$  m/s their size is of the order of 1 mm which is much larger than  $10^{-4}$  mm which is of the order of the gas mean free path. In liquids the smallest eddies are of the order of  $100 \mu\text{m} = 0.1$  mm but the "mean free path" is orders of magnitude smaller than in the gas. Turbulence frequencies vary between  $1\text{s}^{-1}$  and  $10^5\text{s}^{-1}$  while molecular collision frequencies are of the order of  $10^9$  to  $10^{10}\text{s}^{-1}$ .

Laminar mixing is extremely important in a number of polymer processing schemes. If the geometry of the system is known, the flow is strictly laminar and the initial conditions are known, rigorous hydrodynamic models with superimposed diffusion equation can be developed. For details see Ottino et al. Chem. Eng. Sci., 34, 877-890 (1979) and AIChE J., 27, 565-577 (1981) and more recent Ottino's work. The problem, although computationally involved, is doable. Often the key problem is in specifying the initial flow pattern and initial mixture state correctly. Simplified, but useful, approaches in terms of the reduction of the striation thickness to the point where diffusion takes over are also used.

Consider a batch system in state I. Then suddenly expose the fluid to shear motion i.e by moving top plate at velocity,  $\vec{v} = u \frac{y}{L} \vec{e}_x$ . State II is obtained after time  $t$ .

**FIGURE 2:** Snapshot of a single lamella of fluid A exposed to the shear induced by velocity field of eq(1) over time period of  $t$ .



$$\frac{\ell}{\ell_o} = \frac{\frac{L}{ut}}{\sqrt{1 + \left(\frac{L}{ut}\right)^2}} = \frac{1}{\sqrt{1 + \left(\frac{ut}{L}\right)^2}}$$

$$\frac{d\left(\frac{\ell}{\ell_o}\right)}{dt} = \frac{-\frac{u^2}{L^2}t}{\left(1 + \left(\frac{ut}{L}\right)^2\right)^{3/2}}$$

$$\Omega(t) = -\frac{1}{\ell} \frac{d\ell}{dt} = -\frac{d \ln \ell}{dt} = \frac{G^2 t}{1 + G^2 t^2} \quad G = \frac{u}{L} = \frac{\partial v_x}{\partial y}$$

In a good batch mixer one wants to maximize  $\left(-\frac{d \ln \ell}{dt}\right)$  i.e. to maximize the rate of decrease of  $\ell$  w.r.t.  $\ell$ . This maximum occurs when  $t = \frac{L}{u}$  and  $\omega = 45^\circ = \frac{\pi}{4}$ .

An ideal simple shear mixer should operate at this preferred condition by continuously reorienting the fluid. The mixer dissipates energy at a rate per unit volume of

$$\frac{P}{V} = \dot{\epsilon}_v = \mu \left(\frac{dv_x}{dy}\right)^2 = \mu \left(\frac{u}{L}\right)^2 = \mu G^2$$

$$\text{At } t_{\max} = \frac{L}{u} = \frac{1}{G} = \frac{1}{\left(\frac{\partial v_x}{\partial y}\right)}$$

$$\Omega_{\max} = \left(-\frac{d \ln \ell}{dt}\right)_{\max} = \frac{G^2 \frac{1}{G}}{1 + G^2 \frac{1}{G^2}} = \frac{G}{2} = \frac{1}{2} \sqrt{\frac{\dot{\epsilon}_v}{\mu}}$$

Hence, in a shear mixer  $\left(-\frac{d \ln \ell}{dt}\right) \leq \frac{1}{2} \sqrt{\frac{\dot{\epsilon}_v}{\mu}} \leq \frac{1}{2} \sqrt{\frac{\dot{\epsilon}}{\nu}}$  where  $\dot{\epsilon}_v = \dot{\epsilon} \rho$

Ottino shows that in stagnation point flow

$$\Omega_{\max} = \sqrt{\frac{\dot{\epsilon}_v}{2\mu}}$$

This achieves the maximum possible rate of change in striation thickness with power dissipated.

In laminar flow

$$\frac{P}{\rho N^3 d^5} = \frac{C_1 \mu}{d^2 N \rho} = \frac{C}{\text{Re}} \quad N_p = C_1 \text{Re}^{-1}$$

$$P = C_1 \mu N^2 d^3$$

$$\dot{\epsilon}_v = \frac{P}{V} = C_1' \mu N^2 \quad \Omega \propto \sqrt{\frac{\dot{\epsilon}_v}{\mu}} = \sqrt{C_1'} N$$

$$N = \frac{1}{C_1'} \sqrt{\frac{\dot{\epsilon}_v}{\mu}}$$

The representative strain velocity  $\sqrt{\frac{\dot{\epsilon}_v}{\mu}}$  is directly proportional to agitator speed and the rate of reduction of striation thickness is directly proportional to agitator speed (rpm).

Now recall again the definition of

$$\Omega(t) = -\frac{d \ln \ell}{dt}$$

so that

$$-\Omega(t) = \frac{\frac{u^2}{L^2} t}{\left(1 + \frac{u^2}{L^2} t^2\right)}$$

One can show by geometric considerations (see our discussion of the lamellar model for mixing and reaction) that:

$$\frac{\partial v_\ell}{\partial \ell} = \frac{+\frac{u^2}{L^2} t}{\left(1 + \frac{u^2}{L^2} t^2\right)} = -\Omega(t)$$

Thus  $-\Omega(t)$  is the gradient of the velocity component in the direction of striation thickness taken in the direction of the striation thickness. Since  $\Omega(t) > 0$  in our shear flow striation thickness decreases with time but at  $\Omega(t) < 0$  it might increase. This is indirect proof of reversibility when only streamline flow is considered.

Since  $\Omega_{\max} = \sqrt{\frac{\dot{\epsilon}_v}{2\mu}}$  then mixing efficiency can be defined as

$$\eta_{\text{mix}} = \frac{\Omega(t)}{\Omega_{\max}} = \frac{-d \ln \ell / dt}{\sqrt{\dot{\epsilon}_v / 2\mu}}$$

The maximum efficiency then of a simple strain mixer considered here would be

$$(\eta_{\text{mix}})_{\max \text{ strain}} = \frac{\frac{1}{2}}{\frac{1}{\sqrt{2}}} = \frac{1}{\sqrt{2}} = 0.707$$

Higher local mixing efficiencies are possible. Theoretically, in stagnation flows one could achieve  $\eta_{\max} = 1$ . If such efficiency can be maintained at all times

$$\Omega = \sqrt{\frac{\dot{\epsilon}_v}{2\mu}} = -\frac{d \ln \ell}{dt}$$

then the striation thickness decreases exponentially with time:

$$\frac{\ell}{\ell_o} = \exp\left(-\sqrt{\frac{\dot{\epsilon}_v}{2\mu}} t\right)$$

This gives us some incentive to use stagnation flow type mixers, e.g. impinging opposing jets, etc.

Thus, we could in a way let the striation thickness be reduced by folding up to  $\ell_c$  where  $\frac{\ell_c^2}{4D} = \tau_D = 0(\tau_k)$ . Then we consider diffusion and reaction in elements of size  $\ell_c$ .

A better way is to recognize that diffusion is important only in the direction z of striation

thickness  $\ell$ . Then in a Lagrangian system of reference, i.e. following a particular fluid element, we could write an unsteady state balance (z coordinate perpendicular to lamellae).

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial z^2} - v_\ell \frac{\partial c}{\partial z} + R(c)$$

However, since  $\frac{\partial v_\ell}{\partial z} = -\Omega(t)$   
 $v_\ell = -\Omega z$

so that we have

$$\frac{\partial c}{\partial t} - \Omega z \frac{\partial c}{\partial z} = D \frac{\partial^2 c}{\partial z^2} + R(c)$$

One can define a new dimensionless time  $\theta$

$$\theta = D \int_0^t \frac{dt'}{\ell^2}$$

and dimensionless coordinate in the direction of striation thickness

$$\xi = \frac{z}{\ell(t)}$$

This transforms the equation from  $(t, z)$  to  $(\theta, \xi)$  coordinates. Hence,

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \theta} \frac{\partial \theta}{\partial t} + \frac{\partial}{\partial \xi} \frac{\partial \xi}{\partial t} = \frac{D}{\ell^2} \frac{\partial}{\partial \theta} - \frac{z}{\ell^2} \frac{d\ell}{dt} \frac{\partial}{\partial \xi}$$

$$\frac{\partial}{\partial t} = \frac{D}{\ell^2} \frac{\partial}{\partial \theta} + \xi \Omega \frac{\partial}{\partial \xi}$$

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial \theta} \frac{\partial \theta}{\partial z} + \frac{\partial}{\partial \xi} \frac{\partial \xi}{\partial z} = 0 + \frac{1}{\ell} \frac{\partial}{\partial \xi}$$

$$\frac{\partial^2}{\partial z^2} = \frac{1}{\ell} \frac{\partial^2}{\partial \xi^2}$$

$$\frac{\partial}{\ell^2} \frac{\partial c}{\partial \theta} + \xi \Omega \frac{\partial c}{\partial \xi} - \Omega \xi = \frac{D}{\ell^2} \frac{\partial^2 c}{\partial \xi^2} + R(c)$$

$$\frac{\partial c}{\partial \theta} = \frac{\partial^2 c}{\partial \xi^2} + \frac{\ell^2}{D} R(c) \quad (*)$$

$$\text{I.C. } \theta = 0 \begin{cases} -1 \leq \xi \leq 0 & c = 0 \\ 0 \leq \xi \leq 1 & c = c_0 \end{cases}$$

$$\text{B.C. } \xi = \pm \frac{1}{2} \quad \frac{\partial c}{\partial \xi} = 0$$

To solve eq (\*) we must know  $\ell^2$  as a function of  $\theta$ :

→ Stagnation flow mixer

$$\frac{\ell}{\ell_0} = \exp(-\sqrt{\hat{\epsilon}_v / 2\mu} t)$$

$$\ell^2 = \ell_0^2 e^{-2\sqrt{\hat{\epsilon}_v / 2\mu} t}$$

$$\theta = \frac{D}{\ell_0^2} \int_0^t e^{2\sqrt{\hat{\epsilon}_v / 2\mu} t'} dt' = \frac{D \left( e^{2\sqrt{\hat{\epsilon}_v / 2\mu} t} - 1 \right)}{\ell_0^2 2\sqrt{\hat{\epsilon}_v / 2\mu}}$$

$$\ln\left(\frac{\ell_o^2 2}{D} \sqrt{\dot{\epsilon}_v / 2\mu \theta}\right) + 1 = 2\sqrt{\dot{\epsilon}_v / 2\mu} t$$

$$\ell^2 = \ell_o^2 e^{-\ln(\cdot)} = \frac{\ell_o^2}{\frac{\ell_o^2 2\sqrt{\dot{\epsilon}_v / 2\mu \theta}}{D} + 1}$$

$$\frac{\ell^2}{D} = \frac{\ell_o^2 / D}{\frac{\ell_o^2 2\sqrt{\dot{\epsilon}_v / 2\mu} \theta + 1}{D}} \quad \text{Substitute into equation (*)}$$

→ shear flow mixer

$$\ell = \frac{\ell_o}{\sqrt{1 + G^2 t^2}}$$

$$\ell^2 = \frac{\ell_o^2}{1 + G^2 t^2}$$

$$\theta = \frac{D}{\ell_o^2} \int_0^t (1 + G^2 t'^2) dt' = \frac{D}{\ell_o^2} \left[ t + \frac{1}{3} G^2 t^3 \right]$$

$$\theta = \frac{D}{\ell_o^2} t \left( 1 + \frac{1}{3} G^2 t^2 \right) \quad \text{implicit}$$

$$\frac{1}{3} G^2 t^3 = t - \frac{\ell_o^2}{D} \theta = 0$$

$$t^3 + \frac{3}{G^2} t - \frac{3\ell_o^2}{G^2 D} \theta = 0$$

$$a_2 = 0 \quad a_1 = \frac{3}{G^2} \quad a_0 = -\frac{3\ell_o^2}{G^2 D}$$

$$q = \frac{1}{G^2}; r = \frac{1}{G} \left( 0 + 3x \frac{3\ell_o^2 \theta}{G^2 D} \right) = \frac{3\ell_o^2 \theta}{2G^2 D}$$

one real root  $q^3 + r^2 > 0$

$$q^3 = \frac{1}{G^6} \quad r^2 = \frac{9\ell_o^4 \theta^2}{4G^4 D^2}$$

$$s_1 = \left[ \frac{3\ell_o^2}{2G^2 D} + \left( \frac{1}{G^6} + \frac{9\ell_o^4 \theta^2}{4G^4 D^2} \right)^{2/2} \right]^{1/3}$$



$$s_2 = \left[ \frac{3\ell_o^2}{2G^2D} - \left( \frac{2}{G^6} + \frac{9\ell_o^4\theta^2}{4G^4D^2} \right)^{1/2} \right]^{1/3}$$

$$t = s_1 + s_2$$

Substitute  $t = f(\theta)$  in the expression for  $\ell^2$  and use to solve equation (\*).

Similarly, a different expression would result for mixing in other type of flows.

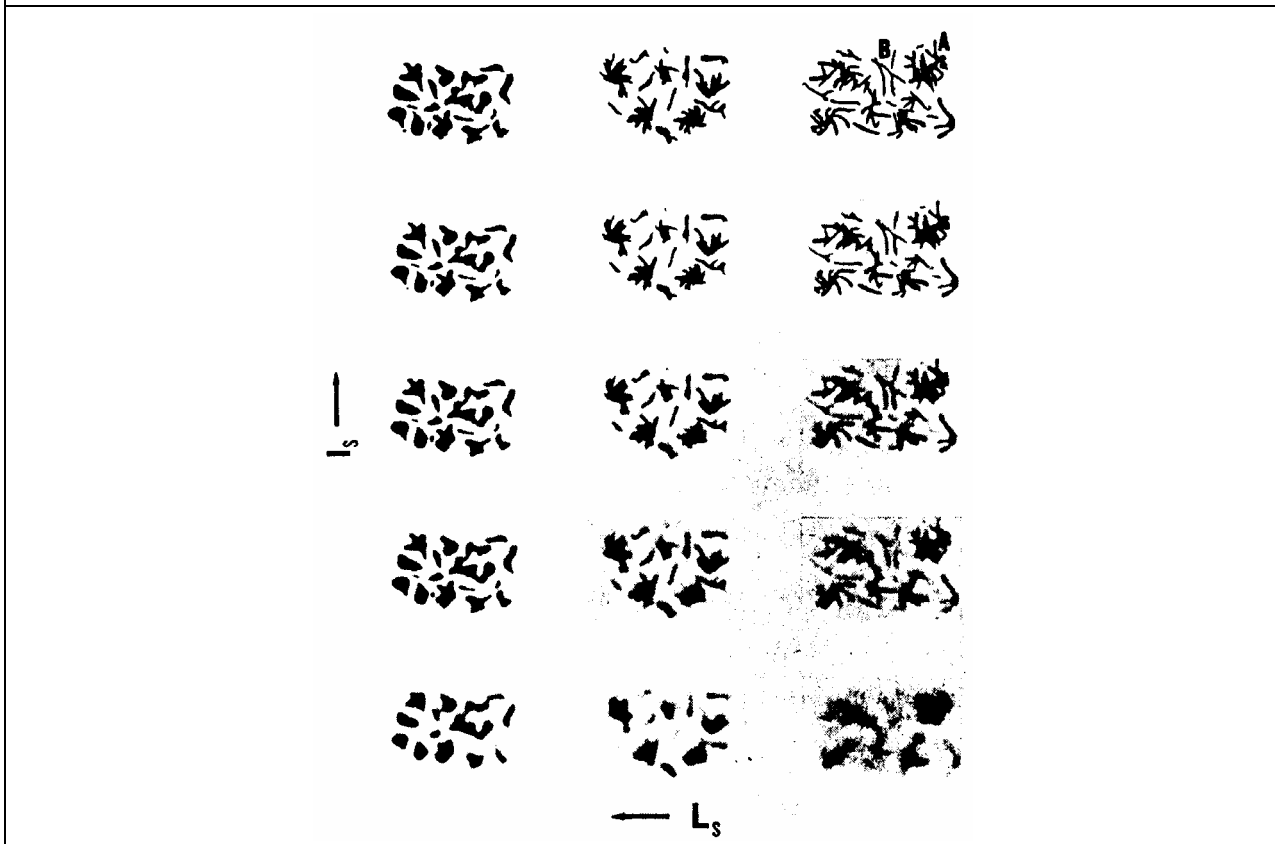
One should note that instead of striation thickness one could also think in terms on interfacial area per unit volume by defining

$$\Omega(t) = -\frac{d \ln \ell}{dt} = \frac{d \ln a_i}{dt}$$

Equations describing the behavior of  $\Omega(t)$  show how the scale of segregation,  $\ell$ , decays or changes in time. Eq (\*) describes how intensity of segregation decays by molecular diffusion even in absence of reaction.

For the example treated above show how the intensity of segregation behaves as a function of time.

Turbulent mixing can probably be best depicted as shown in Figure 3 taken from Brodkey. Following a fluid element the mixing process in time proceeds from the upper left corner to lower right corner. The scale of segregation (striation thickness) is reduced moving from left to right. Intensity of segregation is reduced moving from top to bottom. Both processes occur simultaneously. However, initially when there is little area for diffusion and  $L_s$  is large, reduction in the scale of segregation is important, then at small scale of segregation diffusion dominates. Then the area for diffusion is large and moreover the eddies are already at their smallest size beyond which all dissipation occurs by viscous means. Thus, in the most simplistic, but useful, approach one would need to estimate the characteristic time for macromixing,  $t_m$ , i.e the time required to reduce the scale of segregation to the size,  $l_c$ , where diffusional effects are dominant. Then the microscale for diffusion is  $\tau_m = \ell_c^2 / D$ . If the characteristic kinetic time  $t_k \gg t_m$  then the problem is tractable and the method of solution depends on the ratio of  $\tau_m$  to  $t_k$ . If however  $t_k \leq t_m$  then one has a complex problem when all three processes: reduction of the scale of segregation, reduction of segregation intensity and reaction all occur simultaneously. The only simplification in this class of processes occurs when  $t_k \ll t_m \ll \tau_m$  when reaction occurs on surfaces of the eddies.

**FIGURE 3:** Mechanism of mixing.

### Reynolds Transport Theorem

If  $P$  is property of the system per unit mass (property  $P$  must be conserved),  $\bar{\tau}_p$  is the molecular flux of  $P$  and  $F_p$  is the generation of  $P$  by an external field, then for a volume  $V$  of the fluid medium containing a certain amount of property  $P$  one can write

$$(\text{acc}) = (\text{in}) - (\text{out}) + (\text{generation})$$

$$\frac{d}{dt} \iiint_v P \rho \, dV = - \iint_s \bar{\tau}_p \, d\bar{s} + \iiint_v F_p \, dV$$

Use of Gauss-Ostrogradski's theorem gives

$$\frac{d}{dt} \iiint_v P \rho \, dV = - \iiint_v \nabla \cdot \bar{\tau}_p \, dV + \iiint_v F_p \, dV$$

By Reynolds transport theorem

$$V - \tilde{V} \text{ w.r.t fixed coordinates}$$

$$\frac{\partial(P\rho)}{\partial t} + \nabla \cdot (\bar{v}\rho P) = -\nabla \cdot \bar{\tau}_p + F_p$$

In order to better understand the various approaches in modeling such complex phenomena one needs to get acquainted with the basic notions of turbulence.

First of all in a Euclidian space in the Eulerian description of the flow field (i.e in a coordinate system fixed with respect to some reference point in space) the velocity field is described at each point. A balance on any transferable property P defined per unit mass is given by:

$$\frac{\partial}{\partial t}(\rho P) = -\sum_{j=1}^3 \frac{\partial}{\partial x_j}(u_j \rho P) - \sum_{j=1}^3 \frac{\partial(\tau_p)_j}{\partial x_j} + F_p \quad (1)$$

(accumulation) = (in-out)<sub>by flow</sub> + (in-out)<sub>molecular</sub> + (generation)

$\tau_p$  - transport flux by molecular effects defined as positive in the positive  $x_j$  direction

For example if  $P = 1$ ,  $\tau_p = 0$ ,  $F_p = 0$  eq (1) will yield the total mass balance or the continuity equation. If we want the momentum balance in the i-direction then  $P = u_i$  because  $u_i$  is the momentum per unit mass in the i-th direction. Then

$$(\tau_{u_i})_j = -\sigma_{ji}$$

Thus,  $\sigma_{ji}$  is the stress (force per unit area) in the  $x_i$  direction exerted by the fluid at the positive (upper) side of the surface element perpendicular to the  $x_j$  direction on the fluid on the negative side of this surface element. The stress  $\sigma_{ji}$  is positive if directed in the positive  $x_i$  direction which implies that the molecular momentum flux  $(\tau_{u_i})_j$  is in the negative  $x_j$  direction. For that reason is the convention of the sign introduced.

$\sigma_{ji}$  is a 2nd order tensor (3 x 3 matrix) containing nine components since  $i, j = 1, 2, 3$ .

One readily shows in transport phenomena that the derivatives of the velocity vector components can be expressed in the following form:

$$\frac{\partial u}{\partial x_j} = \frac{1}{2} \underbrace{\left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)}_{\text{component of the } D_{ij} \text{ symmetric deformation tensor}} + \frac{1}{2} \underbrace{\left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right)}_{\text{component of } \Omega_k \text{ vorticity}}$$

or in tensor notation (summation over repeated indices),

$$\frac{\partial u_i}{\partial x_j} = \frac{1}{2} D_{ij} + \frac{1}{2} \Omega_k \varepsilon_{ijk}$$

where

$$\varepsilon_{ijk} = \begin{cases} 0 & \text{two equal indices} \\ 1 & \text{unequal and even perturbation} \\ -1 & \text{unequal and odd perturbation} \end{cases}$$

is the alternating tensor.

For Newtonian fluids only, in tensor notation

$$\sigma_{ji} = -P\delta_{ji} + \mu D_{ji} - \frac{2}{3} \mu \theta \delta_{ji}$$

where  $\delta_{ji} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$  and  $P$  is pressure

$$\theta = \frac{\partial u_i}{\partial x_i} \Rightarrow \sum_{i=1}^3 \frac{\partial u_i}{\partial x_i} = \nabla \cdot \underline{u}$$

non tensor notation

$$\underline{\underline{\sigma}} = \begin{pmatrix} -p + \mu D_{11} - \frac{2}{3} \mu \theta & \mu D_{12} & \mu D_{13} \\ \mu D_{21} & -p + \mu D_{22} - \frac{2}{3} \mu \theta & \mu D_{23} \\ \mu D_{31} & \mu D_{32} & -p + \mu D_{33} - \frac{2}{3} \mu \theta \end{pmatrix}$$

For an incompressible fluid  $\rho = \text{const}$  and  $\theta = 0$ .

For a fluid at isothermal conditions or when there is no change in viscosity due to reaction  $\mu = \text{const}$ .

The i-th momentum balance from eq (1) becomes

$$\rho \frac{\partial u_i}{\partial t} = -\rho \sum_{j=1}^3 \frac{\partial}{\partial x_j} (u_j u_i) + \sum_{j=1}^3 \frac{\partial \sigma_{ji}}{\partial x_j} + F_i$$

$$\sum_{j=1}^3 \frac{\partial}{\partial x_j} (u_j u_i) = u_i \sum_{j=1}^3 \frac{\partial u_j}{\partial x_j} + \sum_{j=1}^3 u_j \frac{\partial u_i}{\partial x_j}$$

$$\begin{aligned}
\sum_{j=1}^3 \frac{\partial \sigma_{ji}}{\partial x_j} &= -\frac{\partial p}{\partial x_i} + \mu \sum_{j=1}^3 \frac{\partial D_{ij}}{\partial x_j} \\
&= -\frac{\partial p}{\partial x_i} + \mu \sum_{j=1}^3 \frac{\partial}{\partial x_j} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \\
&= -\frac{\partial p}{\partial x_i} + \mu \sum_{j=1}^3 \frac{\partial^2 u_i}{\partial x_j^2} + \mu \frac{\partial}{\partial x_i} \sum_{j=1}^3 \frac{\partial u_j}{\partial x_i} \approx 0
\end{aligned}$$

Moreover the substantial derivative can be defined by:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \sum_{j=1}^3 u_j \frac{\partial}{\partial x_j}$$

Then the i-th component of the momentum balance becomes:

$$\rho \frac{Du_i}{Dt} = -\frac{\partial p}{\partial x_i} + \mu \sum_{j=1}^3 \frac{\partial^2 u_i}{\partial x_j^2} + F_i \quad (2)$$

where  $F_i$  is the body force acting in the positive  $x_i$  direction for  $i = 1, 2, 3$  the above represents the usual equations of motion for a Newtonian, incompressible fluid of constant viscosity.

In the turbulent flow field the velocity vector components are customarily decoupled into the time averaged part and fluctuating part

$$U_i = \bar{U}_i + u_i \text{ also } P = \bar{P} + p$$

where

$$\bar{U}_i = \frac{1}{T} \int_0^T U(t + \tau) d\tau$$

and the interval  $T$  is large compared to the reciprocal frequency of turbulent oscillations.

By substituting the average + fluctuating components for the instantaneous values into eq (2) one gets

$$\rho \frac{D(\bar{U}_i + u_i)}{Dt} = -\frac{\partial \bar{P}}{\partial x_i} + \mu \sum_{j=1}^3 \frac{\partial^2 \bar{U}_i}{\partial x_j^2} + F_i + \left[ \mu \sum_{j=1}^3 \frac{\partial^2 u_i}{\partial x_j^2} + f_i - \frac{\partial p}{\partial x_i} \right] \quad (2a)$$

Now we can time average eq (2a) and recall that as long as differentiation and integration can be interchanged (implying continuity of the functions and their derivatives) the average of the average property is the average itself while the average of the fluctuating components is by definition zero since

$$\bar{U}_i = \frac{1}{T} \int_0^T u_i(t+\tau) d\tau = \frac{1}{T} \int_0^T \bar{U}_i d\tau + \frac{1}{T} \int_0^T u_i(t+\tau) d\tau$$

$$\bar{U}_i = \bar{U}_i + \underbrace{\frac{1}{T} \int_0^T u_i(t+\tau) d\tau}_{\bar{u}_i}$$

Hence  $\bar{u}_i = 0$

Then we get

$$\rho \frac{D(\bar{U}_i + u_i)}{Dt} = -\frac{\partial P}{\partial x_i} + \mu \sum_{j=1}^3 \frac{\partial^2 \bar{U}_i}{\partial x_j^2} + \bar{F}_i \quad (3a)$$

We still need to perform the averaging on the left hand side:

$$\begin{aligned} \overline{\frac{D(\bar{U}_i + u_i)}{Dt}} &= \overline{\frac{\partial(\bar{U}_i + u_i)}{\partial t}} + \sum_{j=1}^3 \overline{(U_j + u_j) \frac{\partial(\bar{U}_i + u_i)}{\partial x_j}} = \\ &= \overline{\frac{\partial \bar{U}_i}{\partial t}} + \overline{\frac{\partial u_i}{\partial t}} + \sum_{j=1}^3 \overline{\bar{U}_j \frac{\partial \bar{U}_i}{\partial x_j}} + \sum_{j=1}^3 \overline{\bar{U}_j \frac{\partial u_i}{\partial x_j}} \\ &+ \sum_{j=1}^3 \overline{u_j \frac{\partial \bar{U}_i}{\partial x_j}} + \sum_{j=1}^3 \overline{u_j \frac{\partial u_i}{\partial x_j}} \\ &= \overline{\frac{\partial \bar{U}_i}{\partial t}} + \sum_{j=1}^3 \overline{\bar{U}_j \frac{\partial \bar{U}_i}{\partial x_j}} + \sum_{j=1}^3 \overline{u_j \frac{\partial u_i}{\partial x_j}} \\ &= \overline{\frac{D\bar{U}_i}{Dt}} + \sum_{j=1}^3 \overline{u_j \frac{\partial u_i}{\partial x_j}} \end{aligned} \quad (4)$$

Recall the continuity equation for an incompressible fluid ( $\rho = \text{const}$ ) is:

$$\sum_{j=1}^3 \frac{\partial U_j}{\partial x_j} = 0 \quad \sum_{j=1}^3 \frac{\partial (\bar{U}_j + u_j)}{\partial x_j} = 0 \quad \text{which implies} \quad \sum_{j=1}^3 \frac{\partial \bar{U}_j}{\partial x_j} = 0$$

Then

$$\overline{(\bar{U}_i + u_i) \sum_{j=1}^3 \frac{(\bar{U}_j + u_j)}{\partial x_j}} = 0$$

$$\overline{\bar{U}_i \sum_{j=1}^3 \frac{\partial \bar{U}_j}{\partial x_j}} + \overline{\bar{U}_c \sum_{j=1}^3 \frac{\partial u_j}{\partial x_j}} + \overline{u_i \sum_{j=1}^3 \frac{\partial \bar{U}_j}{\partial x_j}} + \overline{u_i \sum_{j=1}^3 \frac{\partial u_j}{\partial x_j}} = 0$$

$$\bar{U}_i \sum_{j=1}^3 \frac{\partial \bar{U}_j}{\partial x_j} + \overline{u_i \sum_{j=1}^3 \frac{\partial u_j}{\partial x_j}} = 0$$

One can add then  $\overline{u_i \sum_{j=1}^3 \frac{\partial u_j}{\partial x_j}} = 0$  to eq (4) to get:

$$\frac{D(\bar{U}_i + u_i)}{Dt} = \frac{D\bar{U}_i}{Dt} + \sum_{j=1}^3 \frac{\partial}{\partial x_j} (\overline{u_j u_i}) \quad (4a)$$

Substituting (4a) into (3a) we get

$$\rho \frac{D\bar{U}_i}{Dt} = -\frac{\partial \bar{P}}{\partial x_i} + \mu \sum_{j=1}^3 \frac{\partial^2 \bar{U}_i}{\partial x_j^2} - \rho \sum_{j=1}^3 \frac{\partial}{\partial x_j} (\overline{u_i u_j}) + \bar{F}_i \quad (3b)$$

Compare eq (3b) with eq (2). We see that turbulence has introduced another component to the stress tensor due to turbulent fluctuations.

Thus in turbulent flow the stress tensor is modified:

$$(\sigma_{ji})_{\text{turbulent}} = -\bar{P}\delta_{ji} + \mu \bar{D}_{ji} - \underbrace{\rho \overline{u_j u_i}}$$

$-\rho \overline{u_i u_j}$  are Reynolds stresses arising from convective accelerations due to turbulent motion.

$$\overline{u_i u_j} = \frac{1}{T} \int_0^T u_i(t+\tau) u_j(t+\tau) d\tau$$

Recall the definition of  $\sigma_{ji}$  - force per unit area in  $x_i$ -direction executed by momentum transport in negative  $x_j$  direction. Then  $-\rho \overline{u_1^2}$  is the turbulent  $x_1$  momentum executed in the  $+x$  direction.

$-\rho \overline{u_2 u_1}$  is the turbulent momentum in the  $x_1$  direction by momentum transfer from  $x_2$  direction.

The turbulent transport of a scalar property  $\Gamma$ , such as concentration ( $\Gamma = \bar{\Gamma} + \gamma$ ) yields the following set of equations under the same assumptions as made above:

$$\frac{D\bar{\Gamma}}{Dt} = \sum_{j=1}^3 \frac{\partial}{\partial x_j} \left( D \frac{\partial \bar{\Gamma}}{\partial x_j} \right) - \sum_{j=1}^3 \frac{\partial}{\partial x_j} (\overline{u_j \gamma}) + F_\gamma \quad (5)$$

Now a correlation between velocity and concentration fluctuations is needed  $\overline{u_j \gamma}$ .

Two simplified ways to treat with the above problem is through the introduction of the concept of mixing length (Prandtl) or by the use of Bousinesq approximation which introduces apparent "eddy" viscosities and diffusivities by assuming that the turbulent transport is of the gradient type

$$-\overline{u_i u_j} = \nu_t D_{ij} = \nu_t \left( \frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right)$$

$$-\overline{u_i \gamma} = \sum_{j=1}^3 (D_t)_{ij} \frac{\partial \bar{\alpha}}{\partial x_j} = D_t \frac{\partial \bar{\alpha}}{\partial x_i}$$

Although many chemical engineering problems have been approached by this methodology its limitations and flaws are clearly pointed out by:

Hinze, J.O. Turbulence. McGraw Hill 1975

Tennekes, H. and J.L. Lumley. A First Course in Turbulence. MIT Press, 1972.

The problem of the unknown fluctuation quantities can be solved by either representing them as dependent variables by specifying the correlation for their evaluation as functions of known quantities.

Bousinesq concept is used:

$$-\overline{u_i u_j} = \nu_t \left( \frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} k$$

$\nu_t$  - turbulent kinematic viscosity not property of fluid but of turbulence field. The second term of the above expression is not present for incompressible fluids.

1. Zero equation approach

$$\nu_t = C_u \ell^2 \left| \frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right|$$

$\ell$  - mixing length obtainable in some flows from algebraic equation (e.g.  $\ell = 0.4 y$  in pipe flow)

2. One equation approach

$$\nu_t = C_u k^{1/2} \ell$$

$\ell$  - algebraic eq

$$k = \frac{\overline{u^2}}{2} \quad \text{turbulent kinetic energy}$$

$$\frac{Dk}{Dt} = \sum_{i=1}^3 \left[ -\frac{\partial}{\partial x_i} \left( \overline{u_i k} + \frac{1}{\rho} \overline{u_i p} \right) - \sum_{j=1}^3 \overline{u_i u_j} \frac{\partial U_i}{\partial x_j} - \cdot \varepsilon \right]$$

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \sum_{j=1}^3 U_j \frac{\partial}{\partial x_j}$$



3. Two equation approach

$$\nu_t = C_u k^2 / \varepsilon$$

$\varepsilon$  = turbulent energy per unit mass

$k - \varepsilon$  model

$$\ell U_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_i} \right) + \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} - \rho \varepsilon$$

$$\ell U_i \frac{\partial \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu_t}{\sigma_c} \frac{\partial \varepsilon}{\partial x_i} \right) + \frac{C_1 \mu_t \varepsilon}{k} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} - C_2 \frac{\varepsilon^2}{k}$$

Lander & Spalding.

$$C_u = 0.09, C_1 = 1.44, C_2 = 1.92, \sigma_k = 1.0, \sigma_c = 1.3$$

4. Reynolds Stress Equation

Differential equations are specified for all six components of the Reynolds stresses:

$$\langle u_i u_j \rangle$$

Energy Balance

Now we consider the energy balance. Total energy is the sum of kinetic and internal energy if the potential energy due to gravitational field + electromagnetic energy can be neglected. Thus:

$$\varepsilon = \varepsilon_{kin} + \varepsilon_{int} = \frac{1}{2} \sum_{j=1}^3 U_j^2 + \varepsilon_{int}$$

Taking  $P = \varepsilon$  in eq (1) we also realize that

$$(\tau_\varepsilon)_j = - \underbrace{\lambda \frac{\partial T}{\partial x_j}}_{\text{conduction transport}} - \underbrace{\sigma_{ji} U_i}_{\text{energy transport by shear}}$$

$\lambda$  – is conductivity and T is temperature.

For a Newtonian, incompressible fluid we then get

$$\rho \frac{D\varepsilon}{Dt} = \underbrace{\sum_{j=1}^3 \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} \right)}_{\text{(I)}} - \underbrace{\sum_{j=1}^3 U_j \frac{\partial P}{\partial x_j}}_{\text{(II)}} + \underbrace{\sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) U_i \right]}_{\text{(IV)}}$$

I - local change of energy due to accumulation and convective transport

- II - conduction
- III - work due to pressure gradient
- IV - work due to viscous stresses

An internal energy balance is possible based on the first law of thermodynamics and results in:

$$\frac{D\varepsilon_{\text{int}}}{Dt} = \frac{1}{\rho} \sum_{j=1}^3 \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} \right) + \nu \sum_{i=1}^3 \sum_{j=1}^3 \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} \quad (7)$$

(The rate of increase of internal energy) = (net rate of energy transfer by conduction) + (heat generation by viscous dissipation ie work of viscous stresses).

By subtracting eq (7) from eq (6) we get the kinetic energy balance:

$$\frac{D}{Dt} \left( \frac{1}{2} \sum_{j=1}^3 U_j^2 \right) = -\frac{1}{\rho} \sum_{j=1}^3 U_j \frac{\partial P}{\partial x_j} + \sum_{i=1}^3 \sum_{j=1}^3 \left\{ \frac{\partial}{\partial x_j} \left[ \nu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) U_i \right] - \nu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} \right\} \quad (8)$$

where  $\nu = \frac{\mu}{\rho}$

This can be rewritten as:

$$\frac{1}{2} \frac{\partial}{\partial t} \left( \sum_{j=1}^3 U_j^2 \right) = - \sum_{j=1}^3 U_j \frac{\partial}{\partial x_j} \left( \frac{P}{\rho} + \sum_{j=1}^3 \frac{1}{2} U_j^2 \right) \quad (I) \quad (II)$$

$$+ \nu \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_j} \left( U_i \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right) - \nu \sum_{i=1}^3 \sum_{j=1}^3 \left( \frac{U_i u_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} \quad (III) \quad (IV)$$

(Local rate of increase of kinetic energy) = (change in convective transport of pressure and kinetic energy or work done per unit mass and time by the total dynamic pressure) + (work done by viscous stresses) - (work dissipated into heat).

From the above eqs (7) and (8) it is evident that the loss in kinetic energy due to viscous dissipation is the gain in internal energy.

Now introduce the mean and fluctuating components for the turbulent field:

$$U_i = \bar{U}_i + u_i \quad ; \quad P = \bar{P} + p$$

$$\sum_{i=1}^3 U_i^2 = \sum_{i=1}^3 \bar{U}_i^2 + 2 \sum_{i=1}^3 \bar{U}_i u_i + \underbrace{\sum_{i=1}^3 u_i^2}_{q^2}$$

The following procedure can now be followed:

- i) Substitute instantaneous quantities in terms of mean values and fluctuating components into eq (9) and average all terms.
- ii) Multiply eq (3b) with  $\frac{\bar{U}_i}{\rho}$  to get the kinetic energy balance for the mean motion which results in eq (10).

$$\begin{aligned}
 & \frac{1}{2} \frac{\partial}{\partial t} \sum_{j=1}^3 \bar{U}_j^2 + \sum_{j=1}^3 \frac{\partial}{\partial x_j} \bar{U}_j \left( \frac{P}{\rho} + \frac{1}{2} \sum_{i=1}^3 \bar{U}_i^2 \right) = \\
 & \quad (I) \qquad \qquad \qquad (II) \\
 & - \sum_{i=1}^3 \sum_{j=1}^3 \left( \overline{-u_i u_j} \frac{\partial \bar{U}_i}{\partial x_j} \right) + \sum_{j=1}^3 \frac{\partial}{\partial x_j} \left( \overline{-u_i u_j} \bar{U}_i \right) \\
 & \quad (III) \qquad \qquad \qquad (IV) \\
 & + \nu \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_i} \bar{U}_j \left( \frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right) - \nu \sum_{j=1}^3 \sum_{i=1}^3 \left( \frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_i}{\partial x_i} \right) \frac{\partial \bar{U}_i}{\partial x_j} \\
 & \quad (V) \qquad \qquad \qquad (VI)
 \end{aligned} \tag{10}$$

- I - local accumulation of mean motion kinetic energy  
 II - work done by total dynamic pressure

III - work of deformation by turbulent stresses  $i \neq j$   $\text{sgn}(\overline{-u_i u_j}) = \text{sgn}\left(\frac{\partial \bar{U}_i}{\partial x_j}\right)$

Term (III) gives a negative contribution to the kinetic energy of mean motion i.e it extracts energy from the mean motion

- IV - work done by turbulent stresses  
 V - work by viscous stresses  
 VI - viscous dissipation of kinetic energy into heat

Now subtract eq (10) from eq (9) into which substitution as per i) above was made.

$$q^2 = \sum_{i=1}^3 u_i^2$$

The result is the equation for turbulence energy

$$k = \frac{q^2}{2}$$

$$\begin{aligned}
 & \frac{D}{Dt} \left( \frac{1}{2} q^2 \right) = - \sum_{j=1}^3 \frac{\partial}{\partial x_j} \overline{u_j \left( \frac{p}{\rho} + \frac{q^2}{2} \right)} + \sum_{i=1}^3 \sum_{j=1}^3 \left( \overline{-u_i u_j} \frac{\partial \bar{U}_j}{\partial x_i} \right) \\
 & \quad (I) \qquad \qquad \qquad (II) \qquad \qquad \qquad (III) \\
 & + \nu \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_i} \overline{u_j \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)} - \nu \sum_{i=1}^3 \sum_{j=1}^3 \overline{\left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_j}{\partial x_i}} \\
 & \quad (IV) \qquad \qquad \qquad (V)
 \end{aligned} \tag{11}$$

(The change of turbulence energy including convective transport) = (Convective diffusion by turbulence of turbulence mechanical energy or work by the total dynamic pressure of turbulence) + (work of deformation of the mean motion by turbulent stresses) + (work of viscous stresses of turbulent motion) - (viscous dissipation of turbulent motion into heat).

Term (III) appears with opposite signs in eq (10) and eq (11). It extracts the kinetic energy of mean motion and converts it to turbulent energy. Due to interaction between mean motion and turbulent motion energy is extracted from the mean motion through work of deformation by the turbulent stresses, converted to turbulent energy (i.e energy of various size eddies) which ultimately is converted to heat through work of deformation by viscous stresses.

Recall that by our definitions  $-\langle u_i u_j \rangle$  is turbulent momentum transfer in negative j direction. Often

$\text{sgn} \left( -\overline{u_i u_j} \right) = \text{sgn} \left( \frac{\partial \bar{U}_i}{\partial x_j} \right)$ . This means that turbulence will in general decrease in accelerating flows

$\frac{\partial \bar{U}_1}{\partial x_1} > 0$  since  $-\bar{U}_1^2 \frac{\partial \bar{U}_1}{\partial x_1} < 0$ . In decelerating flows turbulence energy increases. A decrease in static P in the flow direction decreases turbulence, an increase, increases it.

Consider now the viscous dissipation term that converts turbulent energy to heat (turbulence energy dissipated per unit mass and unit time).

$$\begin{aligned} \dot{\epsilon} &= \nu \sum_{i=1}^3 \sum_{j=1}^3 \overline{\left( \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_j}{\partial x_i}} \quad (12) \\ &= \nu \sum_{j=1}^3 \overline{\frac{\partial u_1 \partial u_j}{\partial x_j \partial x_i}} + \overline{\frac{\partial u_2 \partial u_j}{\partial x_j \partial x_2}} + \overline{\frac{\partial u_3 \partial u_j}{\partial x_j \partial x_3}} + \overline{\left( \frac{\partial u_j}{\partial x_1} \right)^2} + \overline{\left( \frac{\partial u_j}{\partial x_2} \right)^2} + \overline{\left( \frac{\partial u_j}{\partial x_3} \right)^2} \\ &= \nu \left[ 2 \overline{\left( \frac{\partial u_1}{\partial x_1} \right)^2} + 2 \overline{\left( \frac{\partial u_2}{\partial x_2} \right)^2} + 2 \overline{\left( \frac{\partial u_3}{\partial x_3} \right)^2} + \overline{\left( \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right)^2} + \overline{\left( \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right)^2} + \overline{\left( \frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3} \right)^2} \right] \end{aligned}$$

Also

$$\begin{aligned} \dot{\epsilon} &= \nu \left[ \sum_{j=1}^3 \sum_{i=1}^3 \overline{\left( \frac{\partial u_j}{\partial x_i} \right)^2} + \sum_{j=1}^3 \sum_{i=1}^3 \overline{\frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i}} \right] \\ &= \frac{\nu}{2} \sum_{j=1}^3 \sum_{i=1}^3 \overline{\left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right)^2} + 2\nu \sum_{j=1}^3 \sum_{i=1}^3 \overline{\frac{\partial u_i}{\partial x_i} \frac{\partial u_j}{\partial x_j}} \end{aligned}$$

$$\sum_{k=1}^3 \overline{\omega_k^2} = \frac{1}{2} \sum_{j=1}^3 \sum_{i=1}^3 \left( \overline{\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}}^2 \right)$$

$$\omega_k = -\varepsilon_{ijk} \frac{\partial u_i}{\partial x_j}$$

is the vorticity of turbulence.

Many authors make a vorticity balance too to show that turbulence is rotational in nature. As we see from, eq (12a) the dissipation rate of turbulent mixing is proportional to vorticity fluctuations. An approximate vorticity budget shows that on the average turbulent eddies (vortices) are stretched out. It is vortex stretching that transfers turbulent vorticity (and energy associated with it) from large to small scale fluctuations. By vortex stretching the smallest eddies are continually supplied with energy.

All this resulted in the requirement for numerous fluctuating velocity components correlations in space and time. Thus the problem is formidable.

The first simplification is introduced by assuming that the turbulent field is homogeneous. This means that the statistical properties are the same at any location  $\vec{r}$ . This implies that all spatial derivatives of mean turbulent quantities must be zero.

The turbulence energy equation for spatially homogeneous turbulence takes the form (from eq (11))

$$\frac{\partial}{\partial t} \left( \frac{1}{2} \overline{q^2} \right) = -\nu \sum_{i=1}^3 \sum_{j=1}^3 \overline{\left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_j}{\partial x_i}} \quad (11a)$$

Spatially homogeneous turbulence is a decaying turbulence field and cannot also be stationary.

However, if we assume stationarity of turbulence at least one term must survive in the RHS of eq (11). Typically

$$\sum_{i=1}^3 \sum_{j=1}^3 \overline{-u_i u_j} \frac{\partial \overline{u_j}}{\partial x_i} = \nu \sum_{i=1}^3 \sum_{j=1}^3 \overline{\left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_j}{\partial x_i}} \quad (11b)$$

Nevertheless most frequently homogeneous isotropic turbulence is assumed with respect to the coordinate system moving at the mean velocity of flow. In isotropic turbulence the correlations among fluctuating components are independent of direction. When considering the fate of the smallest viscous dissipating eddies the assumption of isotropy is not so bad because the rate of change of mean properties of flow is slow compared to the rate of change of the smallest eddies.

In a nonisotropic field we have to measure the intensity of turbulence in all 3-directions by

$$\frac{\left( \overline{u_1^2} \right)^{1/2}}{U_1} \quad ; \quad \frac{\left( \overline{u_2^2} \right)^{1/2}}{U_2} \quad \text{and} \quad \frac{\left( \overline{u_3^2} \right)^{1/2}}{U_3}$$

where  $\bar{U}_j$  is the average velocity component in the j direction and  $(\overline{u_j^2})^{1/2}$  is the RMS (root mean square) velocity fluctuation in the j direction. These turbulence intensities range from 0.02 to 0.15 in pipe flow but can be much higher in recirculating flows and turbulent jets. Isotropic turbulence assumption asserts that at least locally  $\overline{u_j^2} = \text{const}$ .

The next important step is to relate turbulent fluctuations that occur:

- i) over the same time period at adjacent locations,
- ii) at identical locations over different time periods.

This is treated rigorously in specialized literature. Here we will give the basic ideas. For an isotropic turbulent field the velocity correlation coefficient in time for a fixed point can be defined as

$$\tilde{R}_t(t) = \frac{\overline{u_t u_{t+\Delta t}}}{u_t^2} \quad (13)$$

where the fluctuating velocity  $u_t$  is measured over a time interval  $\Delta t \gg \Delta \varepsilon$ . Clearly as  $\Delta t \rightarrow 0$ ,  $\tilde{R}_t = 1$ . As  $\Delta t \rightarrow \infty$ ,  $\tilde{R}_t \rightarrow 0$ . This is the autocorrelation coefficient.

It is also possible to compare the fluctuating velocity component at two different points

$$\tilde{R}_r = \frac{\overline{u_z u_{z+r}}}{u_z^2} = f(r) \quad (14)$$

The macroscale of turbulence is then given by

$$L_r = \int_0^{L_{\max}} \tilde{R}_r(r) dr$$

Let us expand  $f(r)$  in Taylor series

$$f(r) = 1 + \frac{r^2}{2} \left( \frac{\partial^2 f}{\partial r^2} \right)_{r=0} + \frac{1}{4!} r^4 \left( \frac{\partial^4 f}{\partial r^4} \right)_{r=0} + \dots$$

by assuming that  $f(r)$  is an even function of  $r$

$$\left( \frac{\partial^2 f}{\partial r^2} \right)_0 = \frac{1}{u_z^2} \overline{u_z \frac{\partial^2}{\partial r^2} (u_z)} = \frac{1}{u_z^2} \left[ \frac{\partial}{\partial r} \left( u_z \frac{\partial u_z}{\partial r} \right)_0 - \overline{\left( \frac{\partial u_z}{\partial r} \right)^2} \right]$$

$$\left( \frac{\partial^2 f}{\partial r^2} \right)_0 = -\frac{1}{u_z^2} \overline{\left( \frac{\partial u_z}{\partial r} \right)^2}$$

$$f(r) = 1 - \frac{r^2}{2u_1^2} \overline{\left(\frac{\partial u}{\partial r}\right)^2} = 1 - \frac{r^2}{\lambda_1^2}$$

Since  $f(r)$  is an approximately parabolic function then its intercept with the abscissa can be approximately obtained by setting  $f(r) = 0$  which happens at  $r = \lambda_1$

$$\lambda_1 = -\frac{2}{\left(\frac{\partial^2 f}{\partial r^2}\right)_0} = \frac{2\overline{u_1^2}}{\left(\frac{\partial u}{\partial r}\right)^2}$$

(15)

$\lambda_1$  is clearly the distance scale of local velocity fluctuations, i.e the scale of micromixing in the  $x_1$  direction.

Let us now denote the contribution to  $\overline{u_1^2}$  of the frequencies between  $n$  and  $n + dn$  to be  $E_1(n)dn$  where

$$\int_0^{\infty} E_1(n) dn = \overline{u_1^2}$$

If we define the total kinetic energy of turbulence per unit mass by  $E_{kt}$

$$E_{kt} = \frac{1}{2} \int_V \overline{q^2} dv = \frac{1}{2} \int_V \sum_{i=1}^3 \overline{u_i^2} dv$$

and we get by integration of eq (11)

$$\frac{dE_{kt}}{dt} = - \int_V \sum_{i=1}^3 \sum_{j=1}^3 \overline{u_i u_j} \frac{\partial \overline{U_j}}{\partial x_i} dV - \nu \int_V \overline{\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \frac{\partial u_i}{\partial x_j}} dV$$

Transition to turbulence can be defined by

$$\frac{dE_{kt}}{dt} = 0$$

For isotropic turbulence it seems

$$E_{kt} = \frac{3}{2} \overline{u_1^2} = \frac{1}{2} \overline{u^2} = \frac{3}{2} \int_0^{\infty} E(n) dn \quad (16)$$

The p.d.f.  $E(n)$  is Taylor's one dimensional energy spectrum given by the Fourier transform of the correlation coefficient  $f(r)$  given by eq (14)

$$E(n) = \frac{4\overline{u_1^2}}{U} \int_0^\infty f(r) \cos\left(\frac{2\pi r}{U}\right) dr$$

$$\frac{1}{\lambda_1^2} = -\frac{1}{2} \left( \frac{\partial^2 f}{\partial r^2} \right)_0 = \frac{\pi^2}{U^2 \overline{u_1^2}} \int_0^\infty n^2 E(n) dn \quad (17)$$

Now one customarily defines a wave number  $k$  instead of frequency  $n$

$$k = \frac{2\pi n}{U}$$

Then after a lot of algebra and by introducing the energy spectrum function  $E(k)$  for isotropic turbulence one can show that

$$\frac{\partial}{\partial t} E(k) = T(k) - 2\nu k^2 E(k)$$

$T(k)$  = transfer of energy in the energy cascade to turbulence.

$$\int_0^\infty T(k) dk = 0$$

$$\dot{\epsilon} = \frac{d}{dt} \int_0^\infty E(k) dk = -2\nu \int_0^\infty k^2 E(k) dk$$

$$E(k) dk = E(n) dn = \frac{-2\nu \cdot 4\pi^2}{U^2} \int_0^\infty n^2 E(n) dn$$

Following key findings in an isotropic turbulent field, there are two scales of dissipation

$$\lambda_f = \lambda_g \sqrt{2}$$

in direction of main flow,  $\lambda_f$ , and  $\lambda_g$  in the transverse direction.

$$\frac{d}{dt} \int_0^\infty E(k, t) dk = -2\nu \int_0^\infty k^2 E(k, t) dk$$

Change in turbulence energy = heat dissipation

$k$  - wave number of turbulence



$$k_1 = 2\pi n / \bar{U}_1 = \text{frequency of turbulence} \propto \frac{1}{\text{eddy size}}$$

high frequency - high wave number - small size

low frequency - low wave number - low size

$k$  = radius vector of the wave number space

$$dk_1 dk_2 dk_3 = k \sin \theta d\phi k d\theta dk$$

$$\dot{\varepsilon} = 6\nu \left[ \overline{\left( \frac{\partial u_1}{\partial x_1} \right)^2} + \overline{\left( \frac{\partial u_1}{\partial x_2} \right)^2} + \overline{\frac{\partial u_1}{\partial x_2} \frac{\partial u_2}{\partial x_1}} \right]$$

$$\dot{\varepsilon} = -15\nu u'^2 \left( \frac{\partial^2 f}{\partial r^2} \right)_o = 30\nu \frac{u'^2}{\lambda_f^2} = 15\nu \frac{u'^2}{\lambda_g^2} = 2\nu \int_0^\infty k^2 E(k, t) dk$$

where  $u' = \sqrt{\bar{u}^2}$

Kolmogoroff's theory of isotropic turbulence leads to the length scale of

$$\eta = \left( \frac{\nu^3}{\dot{\varepsilon}} \right)^{1/4}$$

velocity scale  $v = (\nu \dot{\varepsilon})^{1/4}$

$$\frac{v\eta}{\nu} = 1$$

The wave number where viscous effect is strong is of  $O\left(\frac{1}{\eta}\right)$  i.e.,  $k_d = \frac{1}{\eta}$

Most viscous dissipation occurs there.

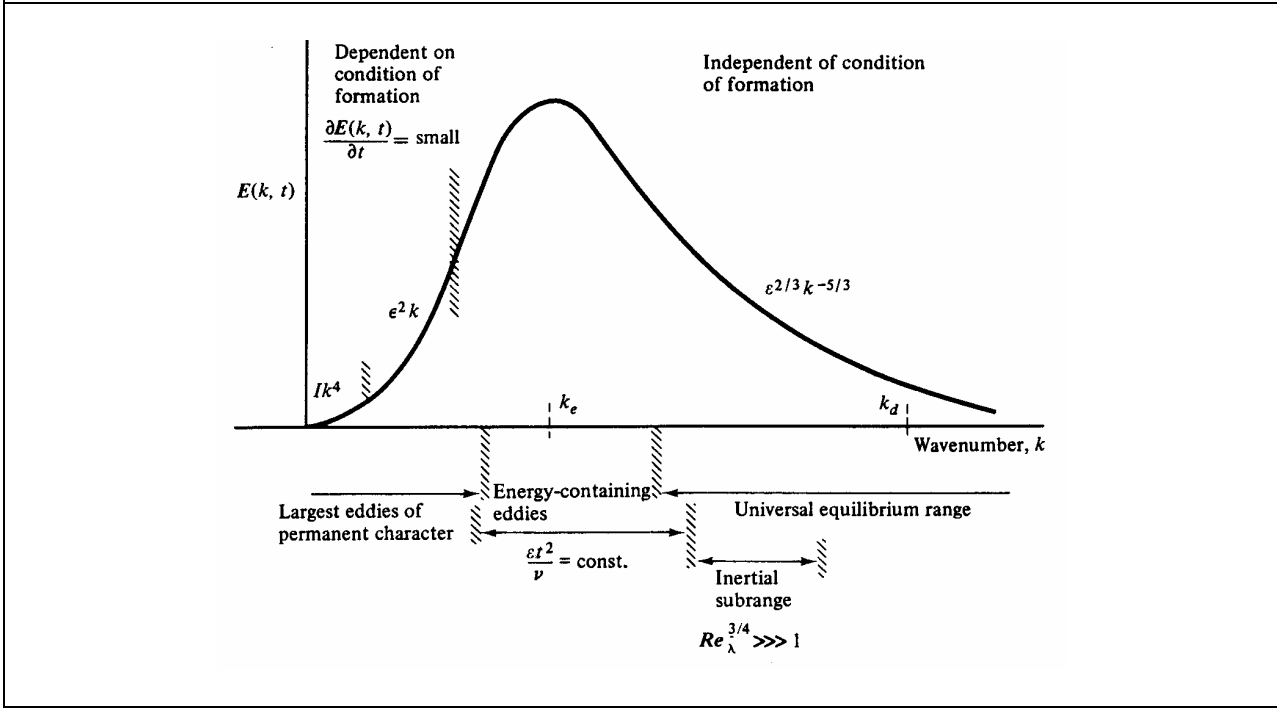
Energy containing eddies have a wave number of  $k_c = \frac{1}{\ell_c}$

Turbulence intensity  $u' = \sqrt{\bar{u}^2}$

Dissipation scale  $\lambda_f$

Integral scale  $\Lambda_f$

**FIGURE 4:** Form of the 3D Energy Spectrum  $E(k, t)$



Decay of isotropic turbulence follows the following equation (recall that  $u' = \sqrt{u'^2}$ )

$$\frac{du'^2}{dt} = -10\nu \frac{u'^2}{\lambda_g^2}$$

The time constant for decay of turbulence intensity is

$$\tau = \frac{\lambda_g^2}{10\nu}$$

$$\dot{\epsilon} = 15\nu u'^2 / \lambda_g^2 \quad \dot{\epsilon} = R\nu t^{-2}$$

$$\frac{du'^2}{dt} = -\frac{2}{3} R\nu t^{-2}$$

For a scalar quantity (say concentration fluctuations  $\gamma'$ ).

$$\frac{d\gamma'^2}{dt} = -12 D \frac{\gamma'^2}{\lambda_\gamma^2} = -\epsilon_\gamma$$

$$\frac{\lambda_\gamma}{\lambda_f} = \frac{\Lambda_\gamma}{\Lambda_f} = \sqrt{\frac{D}{\nu}} = \sqrt{\frac{1}{Sc}}$$

Kolmogoroff's first hypothesis:

At sufficiently high Re there is a range of wave numbers where the turbulence is statistically in equilibrium and uniquely determined by  $\dot{\varepsilon}$  and  $\nu$ . This is a universal equilibrium.

$$\dot{\varepsilon} = -\frac{3}{2} \frac{du'^2}{dt} = 2\nu \int_0^{\infty} k^2 E(k, t) dk$$

At the high Reynolds number the range of energy containing eddies  $k_e$  and the range of maximum viscous dissipation are far apart  $k_e \ll k_d$ .

For  $k \gg k_e$  the rate of energy transferred through the eddies is large compared to the rate of change of their energy - the eddies are in statistical equilibrium.

The total energy supply  $\approx$  total dissipation

$$\dot{\varepsilon} = 2\nu \int_0^{\infty} E(k, t) k^2 dk$$

Assume then that turbulence in this range is uniquely determined by  $\dot{\varepsilon}$  and  $\nu$ . The viscosity scale then by dimensional arguments must be

$$\nu = (\nu \dot{\varepsilon})^{1/4}$$

and

$$\text{Re} = 1 = \frac{u' \eta}{\nu} \quad \eta = \frac{\nu}{u'} = \frac{\nu}{(\nu \dot{\varepsilon})^{1/4}}$$

$$\eta = \left( \frac{\nu^3}{\dot{\varepsilon}} \right)^{1/4} \quad \text{Kolmogoroff scale of turbulence}$$

Turbulence at the Kolmogoroff scale is independent of external conditions,  $k_d = \frac{1}{\eta}$ . This is not the maximum in the dissipation curve. Maximum occurs at  $k\eta \approx 0.5$ .

We also have for energy containing eddies:

$$k_e = \frac{1}{\ell_e}$$

How can one relate this to:  $u', \lambda_f, \Lambda_f$

Define:

$$\text{Re}_\lambda = \frac{u' \lambda_g}{\nu} \quad \text{Re}_\ell = \frac{u' \ell_e}{\nu} \quad \text{turbulent Reynolds number}$$

Equate the dissipation rate to the work per unit time and mass mainly done by large energy containing eddies.

$$\dot{\epsilon} = 15\nu \frac{u'^2}{\lambda_g^2} = A \frac{u'^3}{\ell_e} \quad A = 0(1)$$

Now  $15\nu \frac{u'^2}{\lambda_g^2} = A \frac{u'^3}{\ell_e}$

$$\frac{15\nu}{\lambda_g^2} = A \frac{u'}{\ell_e}$$

$$\frac{u' \lambda_g}{\nu} = \frac{15 \ell_e}{\lambda_g} \Rightarrow \frac{\ell_e}{\lambda_g} = \frac{A}{15} \text{Re}_\lambda$$

Similarly:

$$\text{Re}_\ell = \frac{A}{15} \text{Re}_\lambda^2$$

$$\frac{\lambda_g}{\eta} = 15^{1/4} \text{Re}_\lambda^{1/2}$$

$$\frac{\ell_e}{\eta} = 15^{-3/4} A \text{Re}_\lambda^{3/2}$$

Thus the condition for the existence of the equilibrium range are:

$$k_e \ll k_d \quad , \quad \ell_e \gg \eta$$

$$\text{Re}_\lambda^{3/2} \gg 1 \quad , \quad \text{Re}_\ell^{3/4} \gg 1$$

Kolmogoroff's 2nd hypothesis:

If  $Pe$  is  $\infty$ , the energy spectrum in the subrange  $k_e \leq k \leq k_d$  is independent of  $\nu$  and solely determined by  $\dot{\epsilon}$ . This is the inertial subrange

$$Re_{\lambda}^{3/4} \gg 1 \quad Pe_{\ell} \gg 1$$

Now one moves to the energy containing range (low k). Here,  $t, \epsilon, \nu$  determine turbulence.

$$\frac{\dot{\epsilon} t^2}{\nu} = \text{const} = R - \text{turbulence Reynolds number}$$

This implies that  $R$  remains constant in decaying turbulent fields or that

$$\dot{\epsilon} = R \nu t^{-2}$$

going back to (\*)

$$\frac{du^2}{dt} = -\frac{2}{3} \dot{\epsilon} = -\frac{2}{3} R \nu t^{-2}$$

$$u^2 = C + \frac{2}{3} R \nu t^{-1} = \text{total kinetic energy of turbulence}$$

$$\Lambda_f(t) = \sqrt{2\pi\nu t} \quad \frac{\lambda_f}{\Lambda_f} = \text{const}$$

$$\lambda_f(t) = \sqrt{8\nu t}$$

$$\int_0^{\infty} E(k, t) dk = \frac{3}{2} \int_0^{\infty} E(k, t) dk$$

$$E(k, t) = 8u' \nu^2 t^2 \sqrt{\frac{8\nu t}{\pi}} k^4 e^{-2k^2 \nu t}$$

$$u'^2 = \text{const } t^{-5/2}$$

Turbulence decay

initial, transition, final. If  $M$  = diameter of rod or screen. Inertial period up to  $\frac{x_1}{M} = 100$  to 150;

$$\text{final period } \frac{x_1}{M} > 500 \quad Re_M = \frac{\bar{u}_t M}{\nu} = 650.$$

Initial period  $u^2 = \text{const } t^{-5/2}$

$$u^2 \sqrt{\nu t^5} = \text{const}$$

E(k) changes more rapidly at large k.

For a scalar quantity like the variance of concentration fluctuations the decay law is:

$$\frac{d \overline{c'^2}}{dt} = - 12 \frac{D}{\gamma_i^2} \overline{c'^2}$$

and hence the characteristic time constant for the decay in concentration fluctuation is:

$$\tau_c = \frac{\gamma_i^2}{12 D_m}$$

The characteristic length scale,  $\lambda_c$ , for dissipation of concentration fluctuations has been estimated by

Batchelor as

$$\gamma_c = \gamma_{\text{Batchelor}} = \left( \frac{D \gamma^2}{\dot{\epsilon}} \right)^{1/4}$$

and by Corrsin as

$$\gamma_i = \gamma_{\text{Corrsin}} = \left( \frac{D^3}{\dot{\epsilon}} \right)^{1/4}$$

From actual power spectra Corrsin reported the characteristic time for the decay of the variance of concentration fluctuations as:

$$\tau_c = \left( \frac{5}{\pi} \right)^{2/3} \frac{2}{3 - Sc} \left( \frac{\gamma_s^2}{\dot{\epsilon}} \right)^{1/3}; \quad Sc < 1$$

$$\tau_c = \frac{1}{2} \left\{ 3 \left( \frac{5}{\pi} \right)^{2/3} \left( \frac{\gamma_s^2}{\dot{\epsilon}} \right)^{1/3} + \left( \frac{\gamma}{\dot{\epsilon}} \right)^{1/2} \ln Sc \right\}; \quad Sc > 1$$

where  $\dot{\epsilon}$  is the rate of energy dissipation unit mass and  $\gamma_s$  is the length scale taken by Corrsin to be:

$$\gamma_s = 24 D \left( \frac{L_s^2}{\dot{\epsilon}} \right)^{1/3}$$

where  $L_s$  is the characteristic macro dimension (scale) of the equipment or flow field.